Characterizing the Solubility of Gases in Ionic Liquids Through a Molecular Based Equation of State

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During last decade, the interest in Ionic Liquids (ILs) has increased substantially as can be observed in the large number of publications in the field. The opportunity to apply these substances as an alternative to traditional organic volatile compounds (VOCs) and the development of novel applications in organic chemistry and applied energy has focused the attention of many research groups. Undoubtedly, the understanding of these new systems allowed us the development of new ILs for several applications. Nevertheless, due the large number of ILs and mixtures of them that can be synthesized, much more effort is still required for a systematic development, characterization and fine tuning of desired ILs for final applications. Fast and reliable methods are required in order to study these compounds and the underlying solubility mechanisms of other compounds with different chemical properties. We present here the results concerning the solubility of different gases in a series of alkyl-imidazolium ILs using a molecular-based equation of state, the so called *soft*-SAFT. Two different models for the ILs were developed according to the different structure and chemical properties for the ILs under study. We show that even the complexity of such systems, reasonably simple models are enough to qualitatively describe and predict the phase behavior of these ILs as well as the solubility behavior of some other compounds as hydrogen, carbon dioxide and xenon, in a wide range of thermodynamic conditions.